Claims

Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of the claims in the application. The claims reflect all previous amendments including those introduced by Examiner Allen in the Notice of Allowance dated March 8, 2004. Only claims 1, 69 and 103 are currently amended, and no new matter is introduced by the amendments to the claims, which are being made solely to correct grammatical errors.

Listing of Claims:

1. (Currently amended) A method of predicting a biological activity of a test compound, comprising:

obtaining spectral data for the test compound and for a training set of compounds having known biological activities;

segmenting the spectral data of the training set of compounds into bins;

scaling the segmented spectral data of the training set of compounds prior to establishing a spectral data-activity relationship;

weighting the segmented spectral data of the training set of compounds prior to establishing the spectral data-activity relationship to more heavily weight[[ed]] bins associated with the biological activity;

establishing the spectral data-activity relationship between the known biological activities and the segmented, scaled and weighted spectral data of the training set of compounds using computer implemented pattern recognition;

segmenting the spectral data of the test compound into bins to provide segmented spectral data for the test compound; and

predicting the biological activity of the test compound from the segmented spectral data for the test compound using the spectral data-activity relationship.

2. (Previously presented) The method of claim 1, wherein the spectral data are obtained without first correlating the spectral data with corresponding structural features.

3. (Previously presented) The method of claim 1, wherein the spectral data-activity relationship is established without first correlating the spectral data with corresponding structural features.

4. (Canceled)

5. (Previously presented) The method of claim 1, wherein the spectral data of the test compound is segmented into substantially the same bins as the spectral data of the training set.

6. (Original) The method of claim 1, wherein the spectral data is one type of spectral data.

7. (Previously presented) The method of claim 6, wherein the spectral data is one of nuclear magnetic resonance, mass spectral, infrared, ultraviolet-visible, fluorescence, or phosphorescence data.

8. (Original) The method of claim 1, wherein the spectral data is a composite of different types of spectral data.

9. (Previously presented) The method of claim 8, wherein the composite comprises two or more of the group consisting of nuclear magnetic spectroscopy (NMR), mass spectroscopy (MS), infrared (IR) spectroscopy, and ultraviolet-visible (UV-Vis) spectroscopy.

10. (Previously presented) The method of claim 1, wherein segmenting the spectral data of the test compound comprises segmenting into substantially the same spectral sub-units as the segmented spectral data of the training set of compounds.

11. (Previously presented) A method of predicting a biological activity of a test compound, comprising:

obtaining spectral data for the test compound and for a training set of compounds having known biological activities;

segmenting the spectral data of the training set of compounds into bins;

auto-scaling the segmented spectral data of the training set of compounds prior to establishing a spectral data-activity relationship;

weighting the segmented spectral data of the training set of compounds prior to establishing the spectral data-activity relationship;

establishing the spectral data-activity relationship between the known biological activities and the segmented, scaled and weighted spectral data of the training set of compounds using computer implemented pattern recognition;

segmenting the spectral data of the test compound into bins to provide segmented spectral data for the test compound; and

predicting the biological activity of the test compound from the segmented spectral data for the test compound using the spectral data-activity relationship.

12. (Canceled)

13. (Previously presented) A method of predicting a biological activity of a test compound, comprising:

obtaining spectral data for the test compound and for a training set of compounds having known biological activities;

segmenting the spectral data of the training set of compounds into bins;

scaling the segmented spectral data of the training set of compounds prior to establishing a spectral data-activity relationship;

Fisher-weighting the segmented spectral data of the training set of compounds prior to establishing the spectral data-activity relationship;

establishing the spectral data-activity relationship between the known biological activities and the segmented, scaled and weighted spectral data of the training set of compounds using computer implemented pattern recognition;

segmenting the spectral data of the test compound into bins to provide segmented spectral data for the test compound; and

predicting the biological activity of the test compound from the segmented spectral data for the test compound using the spectral data-activity relationship.

14. (Previously presented) The method of claim 1, wherein establishing and predicting comprises statistical pattern recognition.

Claims 15-16 (Canceled)

17. (Previously presented) A method of predicting a biological activity of a test compound, comprising:

obtaining spectral data for the test compound and for a training set of compounds having known biological activities;

segmenting the spectral data of the training set of compounds into bins;

scaling the segmented spectral data of the training set of compounds prior to establishing a spectral data-activity relationship;

weighting the segmented spectral data of the training set of compounds prior to establishing the spectral data-activity relationship;

establishing the spectral data-activity relationship between the known biological activities and the segmented, scaled and weighted spectral data of the training set of compounds using computer implemented artificial intelligence pattern recognition;

segmenting the spectral data of the test compound into bins to provide segmented spectral data for the test compound; and

predicting the biological activity of the test compound from the segmented spectral data for the test compound using the spectral data-activity relationship and computer implemented artificial intelligence pattern recognition.

18. (Previously presented) A computer implemented method for predicting a biological activity of a test compound, comprising:

receiving spectral data for a test compound as input;

receiving spectral data and endpoint data of a training set of compounds having known biological activities as input;

segmenting the spectral data of the training set of compounds into sub-spectral units;

auto-scaling the segmented spectral data of the training set of compounds;

Fisher-weighting the segmented spectral data of the training set of compounds;

establishing a spectral data-activity relationship between the segmented, scaled and weighted spectral data and the known biological activities of the training set of compounds using pattern recognition;

segmenting the spectral data of the test compound to provide segmented spectral data for the test compound; and

predicting the biological activity of the test compound from the segmented spectral data for the test compound using the spectral data-activity relationship.

19. (Previously presented) The computer implemented method of claim 18, wherein establishing and predicting are performed with a statistical pattern recognition program.

20. (Previously presented) The computer implemented method of claim 19, wherein the spectral data for the test compound is segmented into substantially identical sub-spectral units as the training set spectral data.

21. (Previously presented) The computer implemented method of claim 18, wherein the spectral data are selected from the group consisting of nuclear magnetic resonance data, mass spectral data, infrared data, ultraviolet-visible data, fluorescence data, phosphorescence data, and composites thereof.

22. (Previously presented) The computer implemented method of claim 21, wherein the spectral data-activity relationship comprises canonical variate factors.

23. (Previously presented) The computer implemented method of claim 22, wherein the biological activity is binding affinity to a hormone receptor.

24. (Previously presented) The computer implemented method of claim 23, wherein the spectral data comprise nuclear magnetic resonance data and mass spectral data.

25. (Currently amended) A computer readable medium having stored thereon computer-executable instructions for performing the method of claim 1.

26. (Currently amended) A computer readable medium having stored thereon computer-executable instructions for performing the method of claim 18.

Claims 27-54 (Canceled)

55. (Previously presented) The method of claim 1, wherein the spectral data comprises calculated spectral data.

56. (Previously presented) The computer implemented method of claim 18, wherein the spectral data comprises calculated spectral data.

57. (Previously presented) The computer implemented method of claim 56, wherein the calculated spectral data comprises calculated nuclear magnetic resonance data.

58. (Previously presented) The computer implemented method of claim 57, wherein the calculated nuclear magnetic resonance data comprises calculated ^{13}C NMR data.

Claims 59-64 (Canceled)

65. (Previously presented) A method of predicting a biological activity of a test compound, comprising:

obtaining spectral data for the test compound and for a training set of compounds having known biological activities;

segmenting the spectral data of the training set of compounds into bins;

scaling the segmented spectral data of the training set of compounds prior to establishing a spectral data-activity relationship;

weighting the segmented spectral data of the training set of compounds prior to establishing the spectral data-activity relationship;

establishing the spectral data-activity relationship between known biological activities and the segmented, scaled and weighted spectral data of the training set of compounds using computer implemented pattern recognition;

segmenting the spectral data of the test compound into bins to provide segmented spectral data for the test compound;

predicting the biological activity of the test compound from segmented spectral data for the test compound using the spectral data-activity relationship; and

predicting a second biological activity of the test compound using a second spectral data-activity relationship, the second spectral data-activity relationship established between the scaled and weighted spectral data of a second training set of compounds and the known biological activities of the second training set compounds.

66. (Previously presented) The method of claim 1, wherein the spectral data comprises ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{31}P or ^{35}S NMR data.

67. (Previously presented) The method of claim 66, wherein the spectral data comprises calculated spectral data.

68. (Previously presented) The method of claim 57, wherein the calculated nuclear magnetic resonance data comprises ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{31}P or ^{35}S NMR data.

69. (Currently amended) A method for predicting a biological property of a test compound, comprising:

providing spectral data for a training set of compounds having known biological activities;

providing spectral data for the test compound;

segmenting the spectral data for the test compound into bins to provide segmented spectral data for the test compound;

segmenting the spectral data for the training set of compounds into bins;

scaling the spectral data of the training set of compounds in the bins;

weighting the spectral data of the training set of compounds in the bins to more heavily weight[[ed]] bins associated with the biological property;

establishing a spectral data-activity relationship between the known biological activities and the segmented, scaled and weighted spectral data of the training set of compounds using computer implemented statistical pattern recognition; and

using the spectral data-activity relationship to predict the biological activity of the test compound from the segmented, scaled and weighted spectral data of the test compound.

70. (Previously presented) A method for predicting a biological property of a test compound, comprising:

providing spectral data for a training set of compounds having known biological activities;

providing spectral data for the test compound;

segmenting the spectral data for the test compound into bins to provide segmented spectral data for the test compound;

segmenting the spectral data for the training set of compounds into bins;

auto-scaling the spectral data of the training set of compounds in the bins;

weighting the spectral data of the training set of compounds in the bins;

establishing a spectral data-activity relationship between the known biological activities and the segmented, scaled and weighted spectral data of the training set of compounds using computer implemented statistical pattern recognition; and

using the spectral data-activity relationship to predict the biological activity of the test compound from the segmented spectral data of the test compound.

71. (Previously presented) The method of claim 70, wherein weighting comprises Fisher-weighting.

72. (Previously presented) A method for predicting a biological property of a test compound, comprising:

providing spectral data for a training set of compounds having known biological activities;

providing spectral data for the test compound;

segmenting the spectral data for the test compound into bins to provide segmented spectral data for the test compound;

segmenting the spectral data for the training set of compounds into bins;

scaling the spectral data of the training set of compounds in the bins;

Fisher-weighting the spectral data of the training set of compounds in the bins;

establishing a spectral data-activity relationship between the known biological activities and the segmented, scaled and weighted spectral data of the training set of compounds using computer implemented statistical pattern recognition; and

using the spectral data-activity relationship to predict the biological activity of the test compound from the segmented spectral data for the test compound.

73. (Previously presented) A method for predicting a biological property of a test compound, comprising:

providing spectral data for a training set of compounds having known biological activities;

providing spectral data for the test compound;

segmenting the spectral data for the test compound into bins to provide segmented spectral data for the test compound;

segmenting the spectral data for the training set of compounds into bins;

variance scaling the spectral data of the training set of compounds in the bins;

weighting the spectral data of the training set of compounds in the bins;

establishing a spectral data-activity relationship between the known biological activities and the segmented, scaled and weighted spectral data of the training set of compounds using computer implemented statistical pattern recognition; and

using the spectral data-activity relationship to predict the biological activity of the test compound from the segmented spectral data for the test compound.

74. (Previously presented) A method for predicting a biological property of a test compound, comprising:

providing spectral data for a training set of compounds having known biological activities;

providing spectral data for the test compound;

segmenting the spectral data for the test compound into bins to provide segmented spectral data for the test compound;

segmenting the spectral data for the training set of compounds into bins;

scaling the spectral data of the training set of compounds in the bins;

weighting the spectral data of the training set of compounds in the bins;

establishing a spectral data-activity relationship between the known biological activities and the segmented, scaled and weighted spectral data of the training set of compounds using computer implemented statistical pattern recognition, the spectral data-activity relationship comprising a set of canonical variate factors; and

using the spectral data-activity relationship to predict the biological activity of the test compound from the segmented spectral data for the test compound.

75. (Previously presented) The method of claim 69, wherein the spectral data comprises nuclear magnetic resonance, mass spectral, infrared, ultraviolet-visible, fluorescence, phosphorescence data, or composites thereof.

76. (Previously presented) The method of claim 75, wherein the spectral data comprises ^{13}C NMR data.

77. (Previously presented) The method of claim 76, wherein the ^{13}C NMR data comprises calculated ^{13}C NMR data.

78. (Canceled)

79. (Previously presented) The method of claim 75, wherein the spectral data comprises ^{13}C NMR data and EI-MS data.

80. (Previously presented) The method of claim 69, wherein detecting a pattern comprises statistical pattern recognition.

81. (Previously presented) A method for predicting a biological property of a test compound, comprising:

providing spectral data for a training set of compounds having known biological activities, wherein the spectral data for the training set of compounds comprises ^{13}C NMR data;

providing spectral data for the test compound, wherein the spectral data for the training set of compounds comprises ^{13}C NMR data;

segmenting the spectral data for the test compound into bins to provided segmented spectral data for the test compound, wherein segmenting into bins comprises segmenting the ^{13}C NMR data into bins having a width from 0.5 ppm to 5.0 ppm;

segmenting the spectral data for the training set of compounds into bins, wherein segmenting into bins comprises segmenting the ^{13}C NMR data into bins having a width from 0.5 ppm to 5.0 ppm;

scaling the spectral data of the training set of compounds in the bins;

weighting the spectral data of the training set of compounds in the bins;

establishing a spectral data-activity relationship between the known biological activities and the segmented, scaled and weighted spectral data of the training set of compounds using computer implemented statistical pattern recognition; and

using the spectral data-activity relationship to predict the biological activity of the test compound from the segmented spectral data for the test compound.

82. (Previously presented) A computer implemented method for predicting the biological activity of a test compound, comprising:

receiving as input spectral data for a test compound;

receiving as input training set data, the training data comprising spectral data and biological activities of a training set of compounds;

segmenting the spectral data of the training set into bins;

autoscaling the spectral data of the training set;

Fisher-weighting the spectral data of the training set;

using a pattern recognition method to establish a spectral data-activity relationship that classifies compounds of the training set into two or more endpoint classes from the segmented, autoscaled and Fisher-weighted spectral data of the training set and the biological activities of the training set;

segmenting the spectral data for the test compound into bins to provide segmented spectral data for the test compound; and

using the spectral data-activity relationship to predict the test compound's endpoint class from the segmented spectral data for the test compound.

83. (Previously presented) The computer implemented method of claim 82, wherein the spectral data-activity relationship comprises canonical variate factors for the bins.

84. (Previously presented) The computer implemented method of claim 82, wherein the spectral data of the test compound and the spectral data of the training set of compounds comprise spectral data selected from the group consisting of nuclear magnetic resonance data, mass spectral data, infrared data, ultraviolet-visible data, fluorescence data, phosphorescence data, and composites thereof.

85. (Canceled)

86. (Previously presented) The computer implemented method of claim 84, wherein the spectral data comprises ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{31}P or ^{35}S NMR data.

87. (Previously presented) The method of claim 86, wherein the spectral data is calculated.

88. (Previously presented) The computer implemented method of claim 82, wherein the spectral data of the test compound and the spectral data of the training set of compounds comprise ^{13}C NMR data and segmenting into bins comprises dividing the ^{13}C NMR data into sub-spectral units having a width from 0.5 ppm to 5.0 ppm.

89. (Previously presented) The computer implemented method of claim 88, wherein the ^{13}C NMR data comprises calculated ^{13}C NMR data.

90. (Previously presented) A computer readable medium having stored thereon computer-executable instructions for performing the method of claim 82.

91. (Previously presented) The method of claim 82 further comprising testing the spectral data-activity relationship with a validation set of data.

92. (Previously presented) The method of claim 82 further comprising leave-one-out cross-validating the spectral data-activity relationship.

93. (Previously presented) The method of claim 82, wherein the pattern recognition method is a statistical pattern recognition method.

94. (Previously presented) The method of claim 11, wherein the spectral data comprises ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{31}P or ^{35}S NMR data.

95. (Previously presented) The method of claim 11, wherein the spectral data comprises calculated spectral data.

96. (Previously presented) The method of claim 95, wherein the calculated spectral data comprises ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{31}P or ^{35}S NMR data.

97. (Previously presented) The method of claim 13, wherein scaling comprises variance-scaling.

98. (Previously presented) The method of claim 13, wherein scaling comprises auto-scaling.

99. (Previously presented) The method of claim 13, wherein the spectral data comprises ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{31}P or ^{35}S NMR data.

100. (Previously presented) The method of claim 13, wherein the spectral data comprises calculated spectral data.

101. (Previously presented) The method of claim 100, wherein the calculated spectral data comprises ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{31}P or ^{35}S NMR data.

102. (Previously presented) The method of claim 1, wherein the spectral data of the test compound and the spectral data of the training set of compounds comprise ^{13}C NMR data, and segmenting the spectral data of the training set into bins and segmenting the spectral the test compound into bins comprise dividing the ^{13}C NMR data into sub-spectral units having a width from 0.5 ppm to 5.0 ppm.

103. (Currently amended) A computer-implemented method for predicting a biological activity of a test compound, comprising:

obtaining spectral data for the test compound;

segmenting the spectral data for the test compound into segmented spectral data for the test compound; and

predicting the biological activity of the test compound from the segmented spectral data for the test compound using a spectral data-activity relationship established between segmented, scaled and weighted spectral data and known biological activities for a training set of compounds, wherein the segmented, scaled and weighted spectral data for the training set of compounds is weighted to more heavily weight[[ed]] bins that are associated with the biological activity.

104. (Previously presented) The method of claim 103, wherein the spectral data for the test compound and the segmented, scaled and weighted spectral data for the training set of compounds comprise spectral data selected from the group consisting of nuclear magnetic resonance data, mass spectral data, infrared data, ultraviolet-visible data, fluorescence data, phosphorescence data, and composites thereof.

105. (Previously presented) The method of claim 104, wherein the spectral data for the test compound and the segmented, scaled and weighted spectral data of the training set of compounds comprise calculated spectral data.

106. (Previously presented) The method of claim 105, wherein the calculated spectral data comprises calculated nuclear magnetic resonance data.

107. (Previously presented) The method of claim 106, wherein the calculated nuclear magnetic resonance spectral data comprises calculated ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{31}P or ^{35}S nuclear magnetic resonance data.

108. (Previously presented) The method of claim 106, wherein the calculated nuclear magnetic resonance data comprises calculated ^{13}C NMR data.

109. (Previously presented) The method of claim 103, wherein the segmented spectral data for the test compound and the segmented, scaled and weighted spectral data for the training set of compounds comprise ^{13}C NMR data divided into sub-spectral units having a width from 0.5 ppm to 5.0 ppm.

110. (Previously presented) The method of claim 103, wherein the segmented, scaled and weighted spectral data for the training set of compounds comprises segmented, auto-scaled and weighted data.

111. (Previously presented) The method of claim 110, wherein the segmented scaled and weighed data for the training set of compounds comprises segmented, auto-scaled and Fisher-weighted data for the training set of compounds.

112. (Previously presented) The method of claim 103, wherein the spectral data-activity relationship comprises canonical variate factors.

113. (Previously presented) A computer-implemented method for predicting a biological activity of a test compound, comprising:

obtaining spectral data for the test compound;

segmenting the spectral data for the test compound into segmented spectral data for the test compound; and

predicting the biological activity of the test compound from the segmented spectral data for the test compound using a spectral data-activity relationship established between segmented, auto-scaled and Fisher-weighted spectral data and biological activities of a training set of compounds.

114. (Previously presented) The method of claim 114, wherein the spectral data of the test compound and the segmented, auto-scaled and Fisher-weighted spectral data for the training set of compounds comprise ^{13}C NMR data.